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LARELKIN

Two-body relativistic kinematics code

Version 1.12.1

prepared by

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Summary documentation

Abstract: This interactive and self-explaining computer program allows the relativistic calculation of the kinematics parameters of two-body reactions. Calculations for reactions with masses that are available in the 2012 International Atomic Mass Tables do not require an external input of mass values. Other reactions require the preparation of an appropriate data input file. Together with the FORTRAN95 source file, an executable for MSWindows is provided, and all the auxiliary files, as well.

The package is available online from the IAEA Nuclear Data Section.

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LARELKIN

Two-body relativistic kinematics code

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0. History

The kernel of this program is based on a "FORTRAN IV VERSION OF RUDERMAN'S TWO BODY KINEMATICS PROGRAM" from the year 1969. (J. Davidson, N. Jarmie, and A. Niethammer, "RELKIN: a two-body relativistic kinematics code", Report LA-4349 of the Los Alamos Scientific Laboratory, 18 Dec 1969) consisting of 416 punched cards. Naturally, this program was run as a batch job. In the course of four decades more and more features were included, above all an interactive interface, and for many reactions inside the Periodic System a data base putting an end to the need of supplying mass data externally. Thus a FORTRAN95 compatible code consisting of 27 pages evolved. In acknowledgement of the inclusion of above historic program RELKIN from Los Alamos this code is called LARELKIN.

1. Introduction

Kinematics parameters both of the laboratory and the center-of-mass system are calculated relativistically based on the masses (and excited levels, if any) of the reaction partners, in particular total and kinetic energy, Q-value, momentum, angle, and Jacobian factor. For endothermic reactions the threshold energy is calculated, if double valued, the corresponding energy range. If outgoing particles are emitted (in the lab system) into a (forward) cone, the opening angle of this cone is given, too.

1.1 Input

Most of the input is interactive. Some care was applied to minimize typing. Complicated input, like particle masses, is read from files. Two distinctly different kinds of mass input can be chosen:

1) Use "The Ame2012 atomic mass evaluation (I)" by G.Audi, M.Wang, A.H.Wapstra, F.G.Kondev, M.MacCormick, X.Xu, and B.~Pfeiffer, Chinese Physics C36 p. 1287-1602, December 2012. and "The Ame2012 atomic mass evaluation (II)" by M.Wang, G.Audi, A.H.Wapstra, F.G.Kondev, M.MacCormick, X.Xu, and B.~Pfeiffer, Chinese Physics C36 p. 1603-2014, December 2012. as input for most nuclear reactions within the Periodic Table.

2) In all other cases use an input file prepared earlier to supply the relevant mass values. Its filename has the format A23 and starts with A or N (see Output, below) if this file is generated by the program using the internal mass values, or it starts with I if the file is prepared "by hand" to cover any two-body reaction.

To access both branches in double valued regions (due to kinematic collimation) an additional lab angle outside the cone must be input. Otherwise only the forward branch (in cm) is calculated.

1.2 Output

Aside from the printout file called RELKOUT.txt there is an option to generate individual mass input files for reactions with mass values available from the 2012 International Atomic Mass Table. Their filenames are in format A23, have the extension .par, and start either with A (for atomic masses) or N (for nuclear masses).

Observe that all output files may be overwritten!

Some helpful *comments* on the print out:

the Jacobian factor is $d\sigma_{\text{lab}}/d\sigma_{\text{cm}}$; negative values indicate emission into the back hemisphere

S is the invariant square of the c.m. energy

MQ is the c.m. momentum/rest mass

beta and gamma of the c.m. system with respect to the lab system is also given.

1.2.1 Truncation

The limited numerical resolution requires approximations. E.g., to avoid infinities when converting cm to lab data, 0.00001 deg is used instead of 0 deg (both displayed as 0.00 deg) and 179.99999 deg instead of 180 deg (both displayed as 180.00 deg). This has no experimental relevance and appears harmless enough. However, because of extreme kinematic collimation there will be cases where 179.99999 deg in cm converts to 95 deg in the lab system and 180 deg to 180 deg. Obviously, a strong discrepancy. One must be aware of that because no attempt was made to correct for it as it is utterly irrelevant experimentally. The same applies for the Jacobian factor which can become extremely high (just consider the above explosion of a cm cone with an opening angle of 0.000001 degree into a lab cone with an opening angle of 85 deg (nearly one hemisphere). As these values have no practical use and the bit number of the computer puts a limit to the precision of the calculation, Jacobian factors which are calculated to be in excess of 1.10^{12} are set to zero.

For similar reasons it may happen that some iterations fail near the border of such cones. Over the decades this program was used in connection with neutron work with projectile energies of less than 1000 MeV. For such applications no failure whatsoever was observed.

2. Accuracies

Let us consider the reaction ${}^1\text{H}(n,n){}^1\text{H}$ for projectiles of 1 MeV.

For some it will come as a surprise that elastic scattering of 1 MeV neutrons from hydrogen needs to be calculated relativistically (otherwise scattered energies are about 10^2 eV too large).

2.1 Mass Uncertainties

With $m_n = (1008664.91560 \pm 0.00055)$ $\mu\text{mass units}$ and $m_p = (1007276.46688 \pm 0.00013)$ $\mu\text{mass units}$ we get for $E_n = 1.0000$ MeV at a laboratory angle $\varphi_n = 30.00^\circ$ a best estimate $E_{n\varphi} = (0.74966 \pm 0.00008)$ MeV. The uncertainty stems solely from the (implicit) angle and energy uncertainties because the contributions of the mass uncertainties are utterly negligible.

2.2 Charge State of the Particles

For low Z materials it can be assumed that the interacting nuclei are completely stripped with projectile energies that are much larger than the binding energies (10^1 eV). Therefore, the option of nuclear masses is offered. With high Z materials the degree of stripping will depend on the projectile energy. So, atomic masses, the second option, will only be approximately correct. Considering again scattering of 1 MeV neutrons from hydrogen one finds that at larger angles the Jacobian factor of the outgoing neutron is quite sensitive to the ionization of hydrogen.

3. Description of the Options

3.1 Direct Use of the 2012 International Atomic Mass Table (IAMT)

3.1.1 Sample Terminal Response

default cst=931.494061 MeV/amu

This code calculates relativistically kinematics data of two-body reactions.

Neither IAEA nor the author, M. Drosch, makes any warranty, express or implied, or assumes any liability or responsibility for the use of this software.

Enter: Z, A of projectile, target, outgoing particle

Enter ? for help

3, 7, 2, 4, 3, 7

File name N003007002004003007.par generated

Enter y[es] if you want to use your own mass file

Enter y[es] if you want to use ATOMIC masses

y

Input from 2012 Atomic Mass Tables

Opened mass12.dat

2012

From International Atomic Mass Table:

2 4 He 2424.915610000000

2 4 He 2424.915610000000

3 7 Li 14907.105200000000

3 7 Li 14907.105200000000

Enter y[es] for excited states of the residual nucleus

Enter y[es] if you want to generate an individual mass file

y

Enter filename, a19, for mass file, ".par" is added,

or use A003007002004003007.par by default

Enter y[es] for excited states of the residual nucleus

4He(7Li, 7Li) 4He 2012 atomic masses, uses 931.494061000000

For the 0.0000 MeV level the outgoing particles are in a forward cone

Enter projectile energy (MeV), returns on blank

22.45

Energy step size (MeV), nr. of energies; default is 0.,1

Number of angles, NEGATIVE if C.M.:

10

INPUT of ANGLE values: LINE-BY-LINE or "<enter>" for other OPTIONS

Constant SPACING options: COSINE= 2, DEFAULT= degrees:

Enter MIN. and MAX. angle of RANGE, DEFAULT= full range:

Const. spacing OPTION: RANGE from 0.00 to 180.00 is divided into 9 portions

At 22.450 MeB half opening angle of cone is 34.785 degrees

Enter y[es] if you want to enter additional angles

Enter y[es] if you want to continue with the same reaction

Enter y[es] if you want to continue with the same reaction

Enter y[es] if you want to continue with some other reaction

3.1.2 Sample Output

File A003007002004003007.par:

```
C
  4He( 7Li, 7Li) 4He      2012 atomic masses, uses 931.4940610
      7.00000      4.00000      7.00000      4.00000
16.003436      2.603254      16.003436      2.603254
```

File RELKOUT.txt:

Units of output data:
Energy (MeV)
Angle (degree)
Mass (MeV and/or amu)

```
  4He( 7Li, 7Li) 4He      2012 atomic masses, uses 931.49406 MeV/amu
rest masses incident 6535.3655322( 7.016003436) calculated Q= 0.0000000
      target 3728.4011596( 4.002603254)
      (outgoing) C 6535.3655322( 7.016003436)
      (residual) D 3728.4011596( 4.002603254)
incident lab energy 22.4500 incident lab momentum 542.1641
      CENTER-OF-MASS PARAMETERS:
total energy 10271.9186 beta(c.m.)0.0527 gamma(c.m.) 1.0014 S= 1.055123E+08
part A:tot en 6538.3277 mom 196.7895
part B:tot en 3733.5909 mom 196.7895
part C:tot en 6538.3277 mom 196.7895 beta 0.0301 gam 1.0005 MQ 0.0301
part D:tot en 3733.5909 mom 196.7895 beta 0.0527 gam 1.0014 MQ 0.0528

      particle C      particle D
      cm lab kinetic Jacobian lab kinetic Jacobian
angle angle energy factor angle energy factor
0.00 0.00 22.45000 1.3175E-01 0.00 0.000
56.87 20.00 17.73954 1.3349E-01 61.53 4.710 5.252E-01
180.00 0.00 1.67644-1.7671E+00 0.00 20.774 2.493E-01
163.18 20.00 2.12090-1.1179E+00 8.40 20.329 2.520E-01
```

3.2 Individual Input of Masses using values from the IAMT

The file name of such input files is in format A23, with A (for atomic) or N (nuclear) as the first figure and .par as the last four figures. The file name is generated automatically depending on the input of the Zs and As of projectile, target, and outgoing particle.

Below is a sample of a mass input file. It is important not to terminate data fields with commas because LAHEY FORTRAN95 does not allow that. Observe that the masses are given by the mass number (3rd line) and the mass excess (4th line). The 5th line gives the level energies of the residual particles (in MeV). Their number is given by the fifth value in the third line.

```
C
 12C ( 1 n , 1 n ) 12C      2012 nuclear masses, USES 931.4940610
      1.      12.      1.      12. 4
      8.664916 -3.290375 8.664916 -3.290375
0.      4.43803 7.65420 9.64100
```

3.2.1 Sample terminal response

default cst=931.4940610 MeV/amu

This code calculates relativistically kinematics data of two-body reactions.

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Enter: Z, A of projectile, target, outgoing particle

Enter ? for help

0, 1, 6, 12, 0, 1

File name N000001006012000001.par generated

Enter y[es] if you want to use your own mass file

y

Input from previously prepared mass table

Tries to open N000001006012000001.par

Opened N000001006012000001.par

12C (1 n , 1 n) 12C 2012 nuclear masses, USES 931.4940610

Data file contains 7 levels

0. 4.43803 7.6542 9.641 10.3 10.844 11.828

Enter nr. of levels, start nr. – default is first level

2, 2

Threshold for 4.43803 MeV level is 4.81205 MeV

For the 4.4380 MeV level and projectile energies between threshold and 4.8464 MeV the outgoing particles are in a forward cone

Threshold for 7.65420 MeV level is 8.30037 MeV

For the 7.6542 MeV level and projectile energies between threshold and 8.3597 MeV the outgoing particles are in a forward cone

Enter projectile energy (MeV), returns on blank

15.

Energy step size (MeV), nr. of energies; default is 0.,1

Number of angles, NEGATIVE if C.M.:

-2

INPUT of ANGLE values: LINE-BY-LINE or "<enter>" for other OPTIONS **0.**

45.

Threshold for 4.43803 MeV level is 4.81205 MeV

Threshold for 7.65420 MeV level is 8.30037 MeV

Enter y[es] if you want to enter additional angles

Enter y[es] if you want to continue with the same reaction

y

Enter y[es] if you want to try other excited levels

Enter projectile energy (MeV), returns on blank

15.

Energy step size (MeV), nr. of energies; default is 0.,1

Number of angles, NEGATIVE if C.M.:

-2

INPUT of ANGLE values: LINE-BY-LINE or "<enter>" for other OPTIONS 90.

135.

Threshold for 4.43803 MeV level is 4.81205 MeV

Threshold for 7.65420 MeV level is 8.30037 MeV

Enter y[es] if you want to enter additional angles

Enter y[es] if you want to continue with the same reaction

Enter y[es] if you want to continue with some other reaction

3.2.2 Sample Output

File relkout.txt:

Units of output data:

Energy (MeV)

Angle (degree)

Mass (MeV and/or amu)

```
12C ( 1 n , 1 n ) 12C    2012 nuclear masses,  uses 931.49401 MeV/amu
rest masses  incident   939.5653263( 1.008664916)  calculated Q=  -4.4380300
                target   11174.8631434( 11.996709625)
                (outgoing) C   939.5653263( 1.008664916)
                (residual) D  11179.3011734( 12.001474046)
particle D is in excited state of energy   4.43803
incident lab energy  15.0000    incident lab momentum    168.5585
                CENTER-OF-MASS PARAMETERS:
total energy 12128.2572 beta(c.m.)0.0139 gamma(c.m.) 1.0001 S=  1.470946E+08
part A:tot en  952.3149 mom    155.3082
part B:tot en 11175.9423 mom    155.3082
part C:tot en  948.2249 mom    127.8573 beta  0.1348 gam 1.0092 MQ    0.1361
part D:tot en 11180.0323 mom    127.8573 beta  0.0114 gam 1.0001 MQ    0.0114
```

		particle C		particle D		
cm	lab	kinetic	Jacobian	lab	kinetic	Jacobian
angle	angle	energy	factor	angle	energy	factor
0.00	0.00	10.52812	8.2171E-01	0.00	0.034	-2.160E+01
45.00	41.11	10.00766	8.6273E-01	54.30	0.554	2.133E-01

```
12C ( 1 n , 1 n ) 12C    2012 nuclear masses,  uses 931.49401 MeV/amu
rest masses  incident   939.5653263( 1.008664916)  calculated Q=  -7.6542000
                target   11174.8631434( 11.996709625)
                (outgoing) C   939.5653263( 1.008664916)
                (residual) D  11182.5173434( 12.004926747)
particle D is in excited state of energy   7.65420
incident lab energy  15.0000    incident lab momentum    168.5585
                CENTER-OF-MASS PARAMETERS:
total energy 12128.2572 beta(c.m.)0.0139 gamma(c.m.) 1.0001 S=  1.470946E+08
part A:tot en  952.3149 mom    155.3082
part B:tot en 11175.9423 mom    155.3082
part C:tot en  945.2600 mom    103.6021 beta  0.1096 gam 1.0061 MQ    0.1103
```

part D:tot en 11182.9973 mom 103.6021 beta 0.0093 gam 1.0000 MQ 0.0093

		particle C		particle D		
cm	lab	kinetic	Jacobian	lab	kinetic	Jacobian
angle	angle	energy	factor	angle	energy	factor
0.00	0.00	7.22578	7.8746E-01	0.00	0.120-3.999E+00	
45.00	40.29	6.80406	8.3367E-01	41.72	0.542-5.060E-02	

12C (1 n , 1 n) 12C 2012 nuclear masses, uses 931.49401 MeV/amu
rest masses incident 939.5653263(1.008664916) calculated Q= -4.4380300
target 11174.8631434(11.996709625)
(outgoing) C 939.5653263(1.008664916)
(residual) D 11179.3020534(12.001474046)
particle D is in excited state of energy 4.43803
incident lab energy 15.0000 incident lab momentum 168.5585
CENTER-OF-MASS PARAMETERS:
total energy 12128.2572 beta(c.m.)0.0139 gamma(c.m.) 1.0001 S= 1.470946E+08
part A:tot en 952.3149 mom 155.3082
part B:tot en 11175.9423 mom 155.3082
part C:tot en 948.2249 mom 127.8573 beta 0.1348 gam 1.0092 MQ 0.1361
part D:tot en 11180.0323 mom 127.8573 beta 0.0114 gam 1.0001 MQ 0.0114

		particle C		particle D		
cm	lab	kinetic	Jacobian	lab	kinetic	Jacobian
angle	angle	energy	factor	angle	energy	factor
90.00	84.12	8.75116	9.8437E-01	39.45	1.811 2.565E-01	
135.00	130.51	7.49466	1.1527E+00	20.19	3.067 2.164E-01	

12C (1 n , 1 n) 12C 2012 nuclear masses, uses 931.49406 MeV/amu
rest masses incident 939.5653263(1.008664916) calculated Q= -7.6542000
target 11174.8631434(11.996709625)
(outgoing) C 939.5653263(1.008664916)
(residual) D 11182.5173434(12.004926747)
particle D is in excited state of energy 7.65420
incident lab energy 15.0000 incident lab momentum 168.5585
CENTER-OF-MASS PARAMETERS:
total energy 12128.2572 beta(c.m.)0.0139 gamma(c.m.) 1.0001 S= 1.470946E+08
part A:tot en 952.3149 mom 155.3082
part B:tot en 11175.9423 mom 155.3082
part C:tot en 945.2600 mom 103.6021 beta 0.1096 gam 1.0061 MQ 0.1103
part D:tot en 11182.9973 mom 103.6021 beta 0.0093 gam 1.0000 MQ 0.0093

		particle C		particle D		
cm	lab	kinetic	Jacobian	lab	kinetic	Jacobian
angle	angle	energy	factor	angle	energy	factor
90.00	82.77	5.78592	9.7645E-01	33.69	1.560 1.707E-01	
135.00	129.38	4.76779	1.1893E+00	17.76	2.578 1.655E-01	

3.3 Using an External Mass File for Arbitrary Masses

The file name of such files is in format A23, with I as the first figure. The rest of the file name is arbitrary. The format of the file is like that in 3.2.

3.3.1 Sample terminal response

default cst=931.494061 MeV/amu

This code calculates relativistically kinematics data of two-body reactions.

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Enter: Z, A of projectile, target,
outgoing particle

Enter ? for help

?

Option to enter L for a Z-list of the elements or enter

I for individual input of the mass values, repeat as default

I

Mass values that are not in the International Atomic Mass
Tables are accessible via an individual input file with a
name in format a23 starting with I; enter file name

I000001006012000001.inp

File name I000001006012000001.inp was generated

Input from previously prepared mass table

Tries to open I000001006012000001.inp

Opened I000001006012000001.inp

12C (1 n , 1 n) 12C 2003 nuclear masses, USES 931.4940090

Data file contains 4 levels

0.00000 4.43891 7.65420 9.64100

Enter nr. of levels, start nr. – default is first level

Enter projectile energy (MeV), returns on blank

15.

Energy step size (MeV), nr. of energies; default is 0.,1

1. , 2

Number of angles, NEGATIVE if C.M.:

5

INPUT of ANGLE values: LINE-BY-LINE or "<enter>" for other OPTIONS

Constant SPACING options: COSINE= 2, DEF.= degrees:

Enter MIN. and MAX. angle of RANGE, DEFAULT= full range:

Const. spacing OPTION: RANGE from 0.00 to 180.00 is divided into 4 portions

Enter y[es] if you want to enter additional angles

Enter y[es] if you want to continue with the same reaction

Enter y[es] if you want to continue with some other reaction

3.3.2 Sample output

relkout.txt:

Units of output data:

Energy (MeV)

Angle (degree)

Mass (MeV and/or amu)

```

12C ( 1 n , 1 n ) 12C    2003 nuclear masses,  uses 931.49401 MeV/amu
rest masses  incident  939.5653263( 1.008664916) calculated Q=  0.0000000
              target   11174.8631434( 11.996709625)
              (outgoing) C  939.5653263( 1.008664916)
              (residual) D 11174.8631434( 11.996709625)
incident lab energy  15.0000    incident lab momentum    168.5585
              CENTER-OF-MASS PARAMETERS:
total energy 12128.2572 beta(c.m.)0.0139 gamma(c.m.) 1.0001 S=  1.470946E+08
part A:tot en  952.3149 mom    155.3082
part B:tot en 11175.9423 mom    155.3082
part C:tot en  952.3149 mom    155.3082 beta  0.1631 gam 1.0136 MQ    0.1653
part D:tot en 11175.9423 mom    155.3082 beta  0.0139 gam 1.0001 MQ    0.0139

```

particle C				particle D			
cm	lab	kinetic	Jacobian	lab	kinetic	Jacobian	
angle	angle	energy	factor	angle	energy	factor	
0.00	0.00	15.00000	8.4896E-01	0.00	0.000	8.724E+05	
48.46	45.00	14.27298	8.9097E-01	65.77	0.727	6.092E-01	
94.89	90.00	12.65760	1.0037E+00	42.55	2.342	3.394E-01	
138.45	135.00	11.22613	1.1346E+00	20.77	3.774	2.673E-01	
180.00	180.00	10.68305	1.1947E+00	0.00	4.317	2.500E-01	

```

12C ( 1 n , 1 n ) 12C    2003 nuclear masses,  uses 931.49401 MeV/amu
rest masses  incident  939.5653263( 1.008664916) calculated Q=  0.0000000
              target   11174.8631434( 11.996709625)
              (outgoing) C  939.5653263( 1.008664916)
              (residual) D 11174.8631434( 11.996709625)
incident lab energy  16.0000    incident lab momentum    174.1324
              CENTER-OF-MASS PARAMETERS:
total energy 12129.1786 beta(c.m.)0.0144 gamma(c.m.) 1.0001 S=  1.471170E+08
part A:tot en  953.1639 mom    160.4318
part B:tot en 11176.0147 mom    160.4318
part C:tot en  953.1639 mom    160.4318 beta  0.1683 gam 1.0145 MQ    0.1708
part D:tot en 11176.0147 mom    160.4318 beta  0.0144 gam 1.0001 MQ    0.0144

```

particle C				particle D			
cm	lab	kinetic	Jacobian	lab	kinetic	Jacobian	
angle	angle	energy	factor	angle	energy	factor	
0.00	0.00	16.00000	8.4883E-01	180.00	0.000		
48.46	45.00	15.22412	8.9088E-01	65.77	0.776	6.092E-01	
94.89	90.00	13.50033	1.0038E+00	42.55	2.500	3.394E-01	
138.45	135.00	11.97295	1.1347E+00	20.77	4.027	2.673E-01	
180.00	180.00	11.39353	1.1949E+00	0.00	4.606	2.499E-01	

Appendices

Appendix 1: List of files

Source code:

larelkin.f95

Include file:

param.rel

MSWindows executable:

larelkin.exe

Input files:

disclaimer.txt

elements.txt

mass12.dat

I000001006012000001.inp

Output / Input file:

N000001006012000001.par

A003007002004003007.par

Output file:

relkout.txt

response.log

Appendix 2: List of WARNINGS and ERROR messages (self-explaining)

- ' Input ERROR, repeat input! '
- ' max. allowed levels=',nlev,'!!!! check *.par file'
- ' ERROR when opening ',massfil
- ' ERROR when opening mass12.dat'
- ' possible offset in ethr of: ',df,' MeV'
- 'At E=',f9.5,' MeV all ',i3,' angles outside the cone'
- 'Projectile energy of ',f9.6,' MeV with energy of exc. state=',f9.4,' MeV below threshold of ',f10.6,' MeV'
- 'Attention: sqrt of neg. value avoided '
- 'Attention: neg. value might be serious'

Appendix 3: Acknowledgement and Disclaimer

Originally, this code was prepared by M. DROSG, Faculty of PHYSICS of the UNIVERSITY OF VIENNA, Boltzmannngasse 5, A1090 WIEN AUSTRIA / Europe, for his personal use. In the early seventies N. Jarmie from LASL helped with getting started. His support was very beneficial. Valuable suggestions came from Daniel Abriola, NDS of IAEA. These contributions to this work are thankfully acknowledged.

Neither the author nor anybody else makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of this program and of results obtained by it, or represents that its use would not infringe privately owned rights.

The author will appreciate any comment that will allow improving this program:

E-mail "Manfred.Drosg@UNIVIE.AC.AT"

Vienna, 2017-02-15